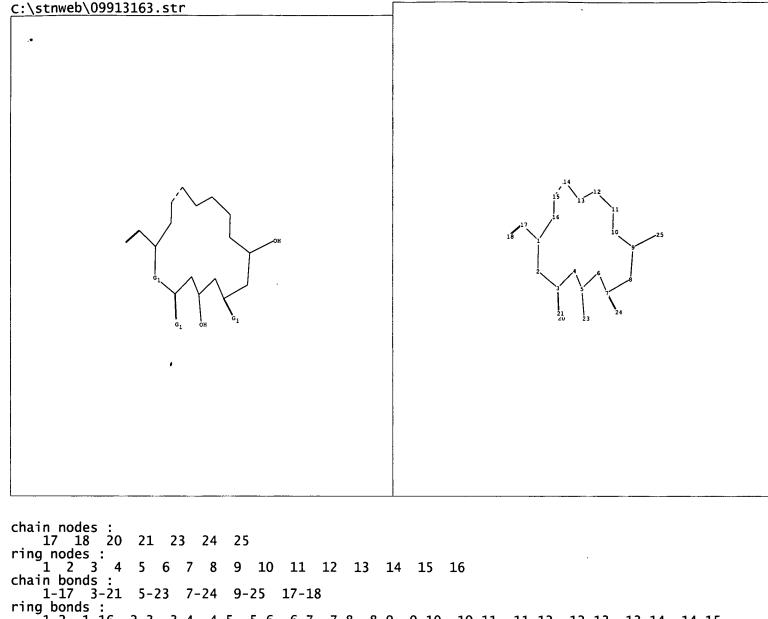


```
chain nodes :
    17   18   26   27   29   30   31
ring nodes :
    1   2   3   4   5   6   7   8   9   10   11   12   13   14   15   16   19   20   21   22   23
chain bonds :
    1-17   3-27   5-29   7-30   9-31   17-18
ring bonds :
    1-2   1-16   2-3   3-4   4-5   5-6   6-7   7-8   8-9   9-10   10-11   11-12   12-13   13-14   14-15
    15-16   19-20   19-23   20-21   21-22   22-23
exact/norm bonds :
    1-2   1-16   1-17   2-3   3-4   3-27   4-5   5-6   5-29   6-7   7-8   7-30   8-9   9-10   9-31   10-11
    11-12   12-13   13-14   14-15   15-16   17-18   19-20   19-23   20-21   21-22   22-23
isolated ring systems :
    containing 1 : 19 :
```

```
Match level:
1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 26:CLASS 27:CLASS 29:CLASS 30:CLASS 31:CLASS
```



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CAS World Wide Web Site (general information)

FILE 'HOME' ENTERED AT 22:58:00 ON 08 SEP 2002

=> file reg

NEWS WWW

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 22:58:14 ON 08 SEP 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 6 SEP 2002 HIGHEST RN 447682-31-7 DICTIONARY FILE UPDATES: 6 SEP 2002 HIGHEST RN 447682-31-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See <u>HELP_CROSSOVER</u> for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> L1

STRUCTURE UPLOADED

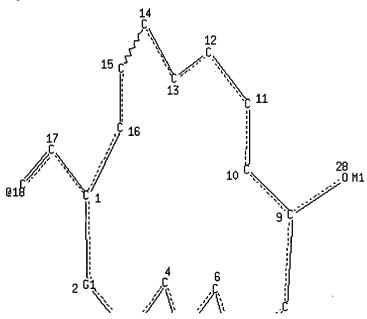
=> d 11

L1 HAS NO ANSWERS

L1 STR

0 29 S 30

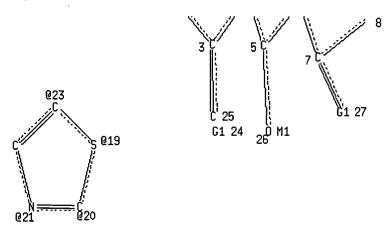
Page 1-A



Page 1-B

@22

Page 2-A



```
Page 2-B
VAR G1=29/30
VPA 18-19/20/21/22/23 S
NODE ATTRIBUTES:
HCOUNT
        IS M1
                   AΤ
                       26
HCOUNT
        IS M1
                   ΑT
                       28
NSPEC
        IS R
                   ΑT
NSPEC
        IS R
                   AΤ
NSPEC
        IS R
                   AΤ
                        3
NSPEC
        IS R
                   ΑT
        IS R
NSPEC
                  ΑT
        IS R
NSPEC
                  ΑT
                        6
                        7
NSPEC
        IS R
                  AΤ
NSPEC
        IS R
                   AΤ
                        8
        IS R
NSPEC
                   ΑT
                        9
        IS R
NSPEC
                  AΤ
                       10
NSPEC
        IS R
                  AT
                       11
NSPEC
        IS R
                  AΤ
                       12
NSPEC
        IS R
                  ΑT
                      13
NSPEC
        IS R
                  AΤ
                      14
NSPEC
        IS R
                  ΑT
                      15
NSPEC
        IS R
                  AΤ
                      16
NSPEC
        IS C
                  AT
                      17
NSPEC
        IS C
                  AT
                       18
NSPEC
        IS R
                      19
                  AT
        IS R
NSPEC
                  ΑT
                       20
        IS R
NSPEC
                  ΑT
                      21
        IS R
NSPEC
                  AT
                      22
        IS R
NSPEC
                  AT
                      23
NSPEC
        IS C
                  ΑT
                      24
NSPEC
        IS C
                  AT
                      25
NSPEC
        IS C
                  AT
                       26
NSPEC
        IS C
                  AT
                       27
NSPEC
        IS C
                  AΤ
                       28
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 17 18 25 26 28 29 30
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
                     30
STEREO ATTRIBUTES: NONE
=> s 11
SAMPLE SEARCH INITIATED 23:04:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                        7 TO ITERATE
100.0% PROCESSED
                        7 ITERATIONS
                                                                  0 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                                 **COMPLETE**
                         ONLINE
                         BATCH
                                  **COMPLETE**
PROJECTED ITERATIONS:
                                  7 TO
                                             298
PROJECTED ANSWERS:
                                  0 TO
                                               0
L2
              O SEA SSS SAM L1
=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 139.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
```

134 TO ITERATE

FULL SEARCH INITIATED 23:04:20 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -

0 ANSWERS

```
100.0% PROCESSED
                        134 ITERATIONS
SEARCH TIME: 00.00.01
L3
                O SEA SSS FUL L1
=>
L4
         STRUCTURE UPLOADED
=> d 14
L4 HAS NO ANSWERS
L4
                  STR
 0 24 S 25
Page 1-A
              15
                        13
                                    11
                  16
                                10
Page 1-B
                      Ĝ1 22
      20
          21<sup>0</sup> M1
    G1 19
Page 2-B
VAR G1=24/25
NODE ATTRIBUTES:
HCOUNT
                         21
         IS M1
                    ΑT
HCOUNT
         IS M1
                         23
                    ΑT
NSPEC
         IS R
                    AT
                          1
NSPEC
                          2
         IS R
                    ΑT
NSPEC
                          3
         IS R
                    AT
NSPEC
         IS R
                    AT
                          4
NSPEC
                          5
         IS R
                    ΑT
NSPEC
         IS R
                    ΑT
                          6
NSPEC
         IS R
                          7
                    ΑT
NSPEC
         IS R
                          8
                    ΑT
                          9
NSPEC
         IS R
                    ΑT
```

10

11

12

AT

ΑT

ΑT

NSPEC

NSPEC

NSPEC

IS R

IS R

IS R

```
NSPEC
        IS R
                  ΑT
                      13
NSPEC
        IS R
                  ΑT
                      14
NSPEC
        IS R
                  AT
                      15
NSPEC
        IS R
                      16
                  AT
NSPEC
        IS C
                  AT
                      17
NSPEC
        IS C
                  AT
                      18
NSPEC
        IS C
                  ΑT
                      -19
NSPEC
        IS C
                  AΤ
                      20
NSPEC
        IS C
                  ΑT
                      21
NSPEC
        IS C
                  AΤ
                      22
NSPEC
        IS C
                  AΤ
                      23
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
                      17. 18' 20 21 23 24 25
DEFAULT ECLEVEL IS. LIMITED :
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
=> s 14
SAMPLE SEARCH INITIATED 23:05:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                    1165 TO ITERATE
 85.8% PROCESSED
                    1000 ITERATIONS
                                                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                                 **COMPLETE**
                         ONLINE
                                 **COMPLETE**
                         BATCH
PROJECTED ITERATIONS:
                              21253 TO
                                          25347
                                  0 TO
PROJECTED ANSWERS:
```

L5 0 SEA SSS SAM L4

=> s 14 full

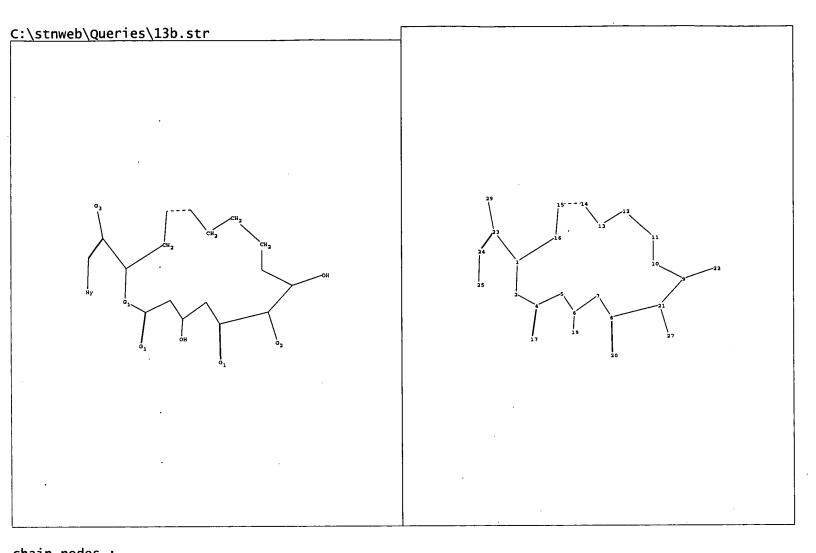
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 139.90 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 23:06:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 22717 TO ITERATE

100.0% PROCESSED 22717 ITERATIONS SEARCH TIME: 00.00.01

0 ANSWERS

L6 0 SEA SSS FUL L4

=>



```
Chain nodes :
    17    19    20    22    23    24    25    27    29

ring nodes :
    1    2    4    5    6    7    8    9    10    11    12    13    14    15    16    21

chain bonds :
    1-23    4-17    6-19    8-20    9-22    21-27    23-24    23-29    24-25

ring bonds :
    1-2    1-16    2-4    4-5    5-6    6-7    7-8    8-21    9-10    9-21    10-11    11-12    12-13    13-14    14-15

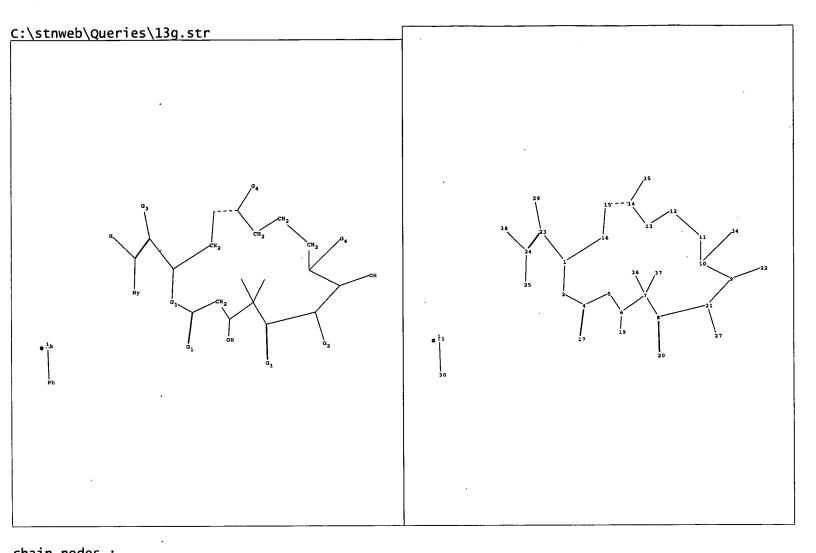
15-16

exact/norm bonds :
    1-2    1-16    1-23    2-4    4-5    4-17    5-6    6-7    6-19    7-8    8-20    8-21    9-10    9-21    9-22    10-11
    11-12    12-13    13-14    14-15    15-16    21-27    23-24    23-29    24-25
```

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:Atom 27:CLASS 29:CLASS



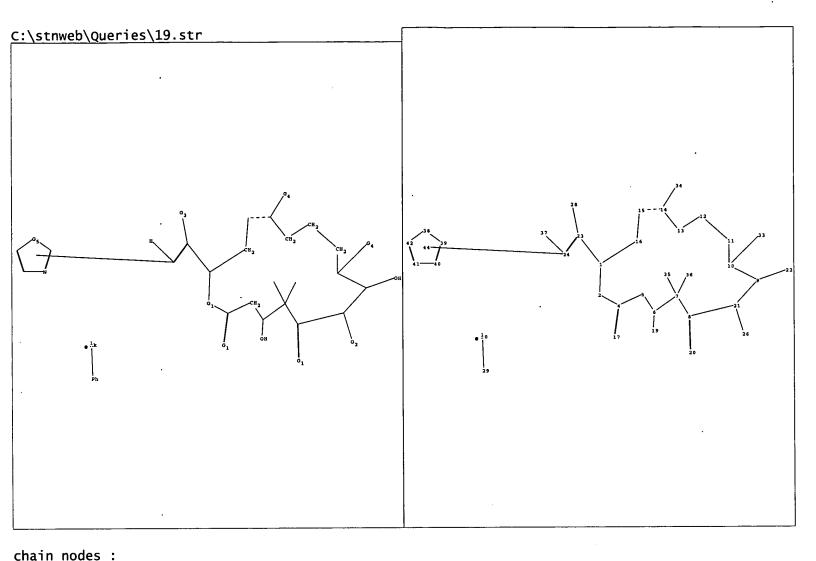
```
chain nodes : 17 19 20 22 23 24
                               25
                                   27
                                        29
                                             30
                                                 31
                                                                   37 38
ring nodes :
    1 2 4 5
                               10 11 12
                                            13 14
                                                     15
                                                          16
chain bonds :
                6-19 7-37 7-36 8-20 9-22 10-34 14-35 21-27 23-24 23-29 24-25 24-38
    1-23 4-17
    30-31
ring bonds :
    1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15
    15-16
exact/norm bonds:
1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-37 7-36 8-20 8-21 9-10 9-21 9-22 10-11 10-34 11-12 12-13 13-14 14-15 14-35 15-16 21-27 23-24 23-29 24-25
    24-38 30-31
G1:0,S
```

G3:H.Ak

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G4: Ph, Ak, H, [*1]

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:Atom 27:CLASS 29:CLASS 30:CLASS 31:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS



```
29
                                             30
    17 19 20
                 22 23 24
                               26
                                   28
                                                 33
ring nodes :
                                                                21
                                                                    38
                                                                                 41 42
    1 2 4 5
                                        12
                                             13
                                                  14
                                                       15
                                                           16
                                10
                                   11
chain bonds :
                6-19 7-36 7-35 8-20 9-22 10-33 14-34 21-26 23-24 23-28 24-37 29-30
    1-23 4-17
ring bonds :
    1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15
    15-16 38-39 38-42 39-40 40-41 41-42
exact/norm bonds :
    1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-36 7-35 8-20 8-21 9-10 9-21 9-22 10-11 10-33 11-12 12-13 13-14 14-15 14-34 15-16 21-26 23-24 23-28 24-37 29-30 38-39 38-42 39-40 40-41 41-42
```

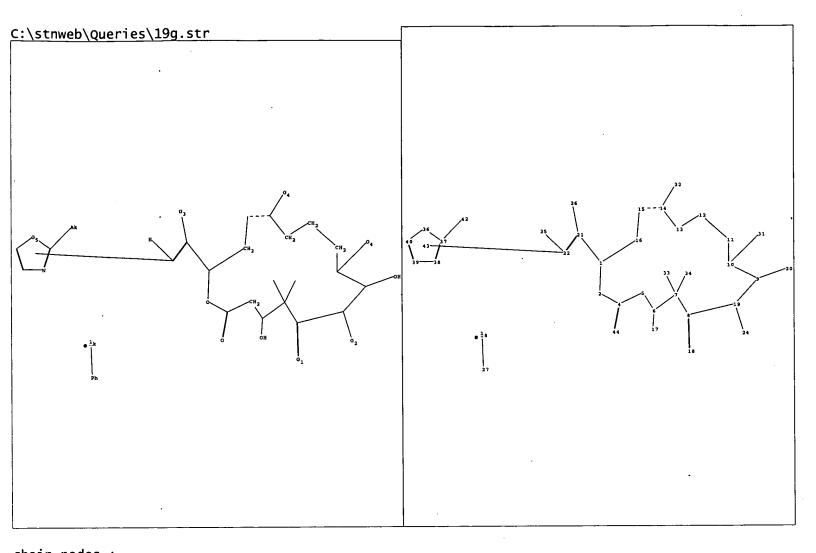
G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak

G4:Ph,Ak,H,[*1]

G5:0,S

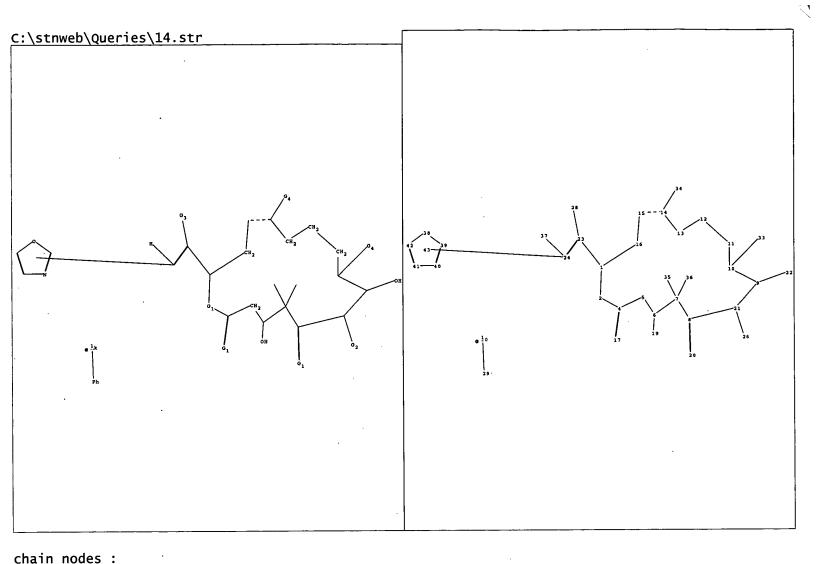
Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 44:CLASS



```
chain nodes :
                                                                          44
    17 18 20
                 21 22 24
                                26 27
                                         28
                                              31
                                                  32
ring nodes :
                                                                     '36
                                                                          37
    1 2 4 5
                                         12
                                              13
                                                   14
                                                       15
                                10
                                    11
chain bonds:
                 6-17 7-34 7-33 8-18 9-20 10-31 14-32 19-24 21-22 21-26 22-35 27-28
    1-21 4-44
    37-42
ring bonds :
    1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-19 9-10 9-19 10-11 11-12 12-13 13-14 14-15
    15-16 36-37 36-40 37-38 38-39 39-40
exact/norm bonds :
    1-2 1-16 1-21 2-4 4-5 4-44 5-6 6-7 6-17 7-8 7-34 7-33 8-18 8-19 9-10 9-19 9-20 10-11 10-31 11-12 12-13 13-14 14-15 14-32 15-16 19-24 21-22 21-26 22-35 27-28 36-37 36-40 37-38 37-42 38-39 39-40
G1:0,S
```

G1:0,S G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu G3:H,Ak G4:Ph,Ak,H,[*1] G5:0,S

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 24:CLASS 26:CLASS 27:CLASS 28:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 42:CLASS 43:CLASS 44:CLASS



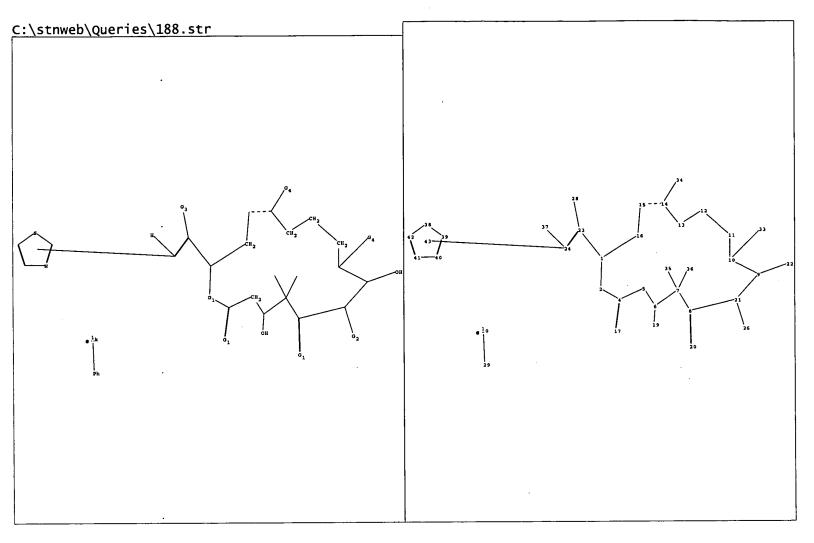
```
28
                                             29
                                                  30
                                                       33
    17 19 20 22 23 24
                                   26
ring nodes :
                                                                      21
                                                                            38
                                                                                 39
                                       11
                                             12
                                                  13
                                                       14
                                                            15
                                                                 16
     1 2 4 5
                                   10
chain bonds :
     1-23 4-17 6-19 7-36 7-35 8-20 9-22 10-33 14-34 21-26 23-24 23-28 24-37 29-30
ring bonds:
     1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21 9-10 9-21 10-11 11-12 12-13 13-14 14-15 15-16 38-39 38-42 39-40 40-41 41-42
exact/norm bonds :
    1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-36 7-35 8-20 8-21 9-10 9-21 9-22 10-11 10-33 11-12 12-13 13-14 14-15 14-34 15-16 21-26 23-24 23-28 24-37 29-30 38-39 38-42 39-40 40-41 41-42
```

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak

G4: Ph, Ak, H, [*1]

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS



```
chain nodes :
    17 19 20 22 23 24
                                   26 28 29
                                                  30 33
                                                            34
                                                                 35
ring nodes :
                                                                                 39 40 41 42
                                                      14 15
                                                                      21
                                                                            38
    1 2 4 5
                   6 7 8
                                   10 11 12
                                                  13
                                                                  16
chain bonds :
    1-23 \quad 4-17 \quad 6-19 \quad 7-36 \quad 7-35 \quad 8-20 \quad 9-22 \quad 10-33 \quad 14-34 \quad 21-26 \quad 23-24 \quad 23-28 \quad 24-37 \quad 29-30
ring bonds :
     1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-21
                                                          9-10 9-21 10-11 11-12 12-13 13-14 14-15
     15-16 38-39 38-42 39-40 40-41 41-42
exact/norm bonds :
    1-2 1-16 1-23 2-4 4-5 4-17 5-6 6-7 6-19 7-8 7-36 7-35 8-20 8-21 9-10 9-21 9-22 10-11 10-33 11-12 12-13 13-14 14-15 14-34 15-16 21-26 23-24 23-28 24-37 29-30 38-39 38-42 39-40 40-41 41-42
```

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak

G4:Ph,Ak,H,[*1]

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS

```
C:\stnweb\Queries\14s.str
```

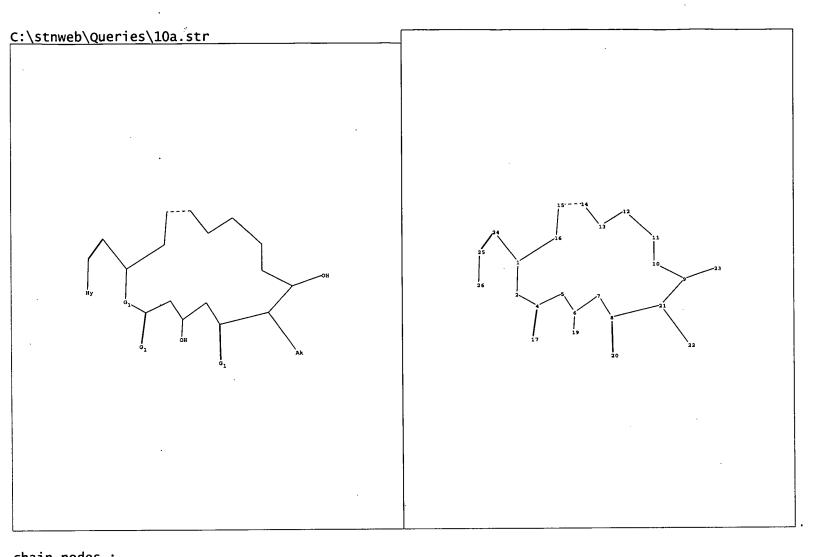
```
chain nodes :
   17 18 20
               21 23 25
                            26
                                27
                                    30
                                         31
                                            32
                                                 33
ring nodes :
                                                              37
                                                                  38
                                                                      39
   1 2 4 5
                                    12
                                         13
                                             14
                                                 15
                                                         19
                            10
                                11
chain bonds :
                                        9-20 10-30 14-31 19-23 21-25 21-43 26-27 34-43
   1-21 4-36 6-17 7-33 7-32 8-18
ring bonds :
    1-2 1-16 2-4 4-5 5-6 6-7 7-8 8-19
                                              9-10 9-19 10-11 11-12 12-13 13-14 14-15
    15-16 37-38 37-42 38-39 39-40 40-41 41-42
exact/norm bonds :
  1-2 1-16 2-4 4-5 4-36 5-6 6-7 6-17 7-8 8-18 8-19 9-10 9-19 9-20 10-11 10-30 11-12 12-13 13-14 14-15 14-31 15-16 19-23 21-25 26-27
exact bonds :
   1-21 7-33 7-32 21-43 34-43
normalized bonds : 37-38 37-42 38-39 39-40 40-41 41-42
G1:0,S
G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu
```

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 19:Atom 20:CLASS 21:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:CLASS 43:CLASS 44:CLASS

G3:H,Ak

G5:0,S

G4:Ph,Ak,H,[*1]



```
chain nodes :
    17    19    20    22    23    24    25    26

ring nodes :
    1    2    4    5    6    7    8    9    10    11    12    13    14    15    16    21

chain bonds :
    1-24    4-17    6-19    8-20    9-23    21-22    24-25    25-26

ring bonds :
    1-2    1-16    2-4    4-5    5-6    6-7    7-8    8-21    9-10    9-21    10-11    11-12    12-13    13-14    14-15
    15-16

exact/norm bonds :
    1-2    1-16    1-24    2-4    4-5    4-17    5-6    6-7    6-19    7-8    8-20    8-21    9-10    9-21    9-23    10-11
    11-12    12-13    13-14    14-15    15-16    21-22    24-25    25-26
```

Match level:
1:Atom 2:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom

```
C:\stnweb\queries\163c.str
```

```
chain nodes :
    18 19 20 21 22 23
                                  30 31 32
ring nodes :
    1 2 3
42 43
                                                                                                      39 40 41
                   5 6 7
                                                    13 14 15 16 24 25 26 27
                                                                                           28
                                                                                                 38
                                     10
                                          11 12
chain bonds :
    1-22 8-35 9-20 10-46 11-19 13-21 15-18 22-23 22-30 23-27 31-32 37-41
    1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-16 24-25 24-28 25-26 26-27 27-28 38-39 38-43 39-40 40-41 41-42 42-43
exact/norm bonds :
    1-2 1-16 1-22 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-35 9-10 9-20 10-11 10-46 11-12 11-19 12-13 13-14 13-21 14-15 15-16 15-18 22-23 22-30 23-27 24-25 24-28 25-26 27 27-28 31-32 37-41
normalized bonds :
    38-39 38-43 39-40
                              40-41 41-42 42-43
isolated ring systems :
    containing 24:
```

G1:0,S G2:H,Ak G3:H,Cb,Ak,[*1] G4:Ak,[*2]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 30:CLASS 31:Atom 32:CLASS 35:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 46:CLASS

```
C:\stnweb\Queries\163a.str
```

```
18 19 20 21 22 23 30 31 32 35 36

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 24 25 26 27 28

chain bonds:

1-22 4-36 8-35 9-20 11-19 13-21 15-18 22-23 22-30 23-27 31-32

ring bonds:

1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-16 24-25 24-28 25-26 26-27 27-28

exact/norm bonds:

1-2 1-16 1-22 2-3 3-4 4-5 4-36 5-6 6-7 7-8 8-9 8-35 9-10 9-20 10-11 11-12 12-13 13-14 13-21 14-15 15-16 15-18 22-23 22-30 23-27 24-25 24-28 25-26 26-27 27-28 31-32

isolated ring systems:

containing 24:
```

G2:H,Ak

G3:H,Cb,Ak,[*1]

chain nodes :

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 30:CLASS 31:Atom 32:CLASS
35:CLASS 36:CLASS

```
C:\stnweb\Queries\613b.str
```

```
1-22 8-35 9-20 10-46 11-19 13-21 15-18 22-23 22-30 23-27 25-47 31-32 37-41
ring bonds :
     1-2 1-16 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15
     15-16 24-25 24-28 25-26 26-27 27-28 38-39 38-43 39-40 40-41 41-42 42-43
exact/norm bonds :
     1-2 1-16 1-22 2-3 3-4 4-5 5-6 6-7 7-8 8-9 8-35 9-10 9-20 10-11 10-46 11-12 11-19 12-13 13-14 13-21 14-15 15-16 15-18 22-23 22-30 23-27 24-25 24-28 25-26 25-47 26-27 27-28 31-32 37-41
normalized bonds:
_38-39 38-43 39-40
                                   40-41 41-42 42-43
isolated ring systems :
     containing 24:
G1:0,S
G2:H,Ak
G3:H,Cb,Ak,[*1]
G4:Ak,[*2]
Match level:
     1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 30:CLASS 31:Atom 32:CLASS 35:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 46:CLASS
      47:CLASS
```

chain nodes :

ring nodes : 1 2 3 42 43

chain bonds :

18 19 20 21 22 23

30 31 32

4 5 6 7 8 9 10 11 12

35

37

13 14 15 16 24 25 26

39 40 41

27

28

38